数理解析研究所講究録
第 1997 巻 2016 年 133-139

A two-scale model for concrete carbonation process in a three dimensional domain

日本女子大学・理学部 愛木豊彦 (Toyohiko Aiki)
Department of Mathematical and Physical Sciences, Faculty of Science
Japan Women's University

名城大学・理工学部 村瀬勇介 (Yusuke Murase)
Department of Mathematics, Faculty of Science and Technology
Meijo University

長岡工業高等専門学校・一般教育科 佐藤直紀 (Naoki Sato)
Division of General Education
Nagaoka National College of Technology

苫小牧工業高等専門学校・総合学科 熊崎耕太 (Kota Kumazaki)
Department of Natural and Physical Sciences
Tomakomai National College of Technology

1 Introduction

Concrete carbonation is one of important issues in our real life so that it is necessary to elucidate its dynamics. On this subject Muntean-Böhm already proposed a free boundary model on a one-dimensional interval in [19, 21], and we studied the simplified model for their one and established large-time behavior of the free boundary in [4, 5, 6, 7].

The main topic of this paper is concerned with the mathematical model for concrete carbonation in a three-dimensional domain, which was given by Maekawa-Chaube-Kishi[17] and Maekawa-Ishida-Kishi[18] from a civil engineering point of view. The model consists of the moisture transport equation and the diffusion equation for carbon dioxide. In this paper we deal with only the former equation and the latter one was discussed in [13, 14, 15].

Here, we show our first model for moisture transport, briefly, since the detail of the modeling was mentioned in [1]. We suppose that the concrete occupies the bounded domain $\Omega \subset \mathbb{R}^3$ with the smooth boundary. Let ρ_w be the density of water, s be the degree of saturation and h be the relative humidity. From observations for real experimental results it is pointed out that the graph of the relationship between s and h is close to one of hysteresis with anti-clockwise trend in [17, 18]. Accordingly, from a phenomenological point of view we approximated the relationship with a play operator in [2, 3, 1, 16]. Then we obtain the following system:

$$\rho_w h_t - \text{ div } (g(h)\nabla h) = sf \quad \text{in } Q(T) := (0,T) \times \Omega, \tag{1.1}$$

$$s_t + \partial I(h; s) \ni 0 \quad \text{in } Q(T), \tag{1.2}$$

$$h = h_b \quad \text{on } \Gamma(T) := (0,T) \times \partial\Omega, \tag{1.3}$$

$$h(0) = h_0, s(0) = s_0 \quad \text{on } \Omega, \tag{1.4}$$

where f is a given function on $Q(T)$ and indicates the generation of water by the chemical reaction, h_b and h_0 be given function on $Q(T)$ and Ω, respectively, and g is a continuous function on $(0,\infty)$ (see Figure 1) and describes the diffusion coefficient depending on the humidity. The ordinary differential equation (1.2) is one of characterization for the play operator (see [10, 25] and Figure 2), and I is the indicator function of the closed interval $[f_*(h), f^*(h)]$ and ∂I is its subdifferential, where f_* and f^* are lower and upper branches of the hysteresis loop, respectively.

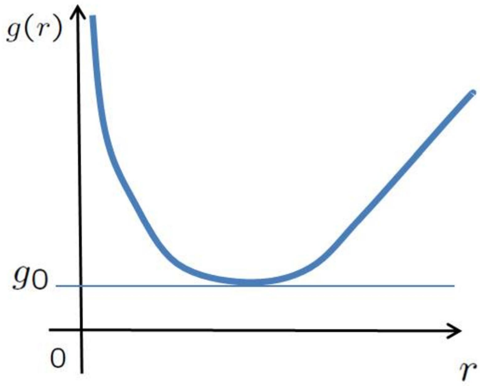

Figure 1: Diffusion coefficient

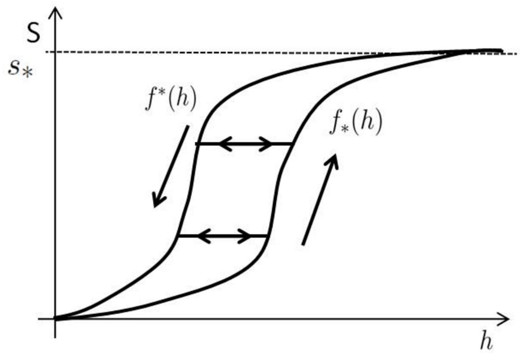

Figure 2: Graph of play operator

For the system (1.1) $\sim$ (1.4) (:= CP) we already proved:

Theorem 1.1. *([2, 3, 16])*
(A1) $g \in C^2((0,\infty))$, $g(r) \geq g_0$ *for* $r > 0$, *where* g_0 *is a positive constant.*
(A2) $f \in L^\infty(Q(T))$, $f_t \in L^2(0,T;L^2(\Omega))$ *and* $f \geq 0$ *a.e. on* $Q(T)$.
(A3) $f_*, f^* \in C^2(\mathbb{R}) \cap W^{2,\infty}(\mathbb{R})$, $0 \leq f_* \leq f^* \leq s_*$, *where* s_* *is a positive constant.*
(A4) $h_b \in C^{2,1}(\overline{Q(T)})$, $h_{bt} \in L^2(0,T;H^2(\Omega))$, $h_b \geq \delta_0 > 0$ *a.e. on* $\Gamma(T)$, $h_0 \in H^2(\Omega) \cap W^{1,\infty}(\Omega)$, $s_0 \in H^1(\Omega) \cap L^\infty(\Omega)$, $h_0 \geq \delta_0$ *a.e. on* Ω, $h_b(0) = h_0$ *a.e. on* $\partial\Omega$, $f_*(h_0) \leq s_0 \leq f^*(h_0)$ *a.e. on* Ω, *where* δ_0 *is a positive constant.*
If (A1) $\sim$ *(A4) hold, then CP has a unique solution on* $[0,T]$.

As a next step of this research we will consider the following equation as a mathematical description for moisture transport:

$$\rho_w h_t - \text{ div } ((g(h) + \phi(1-s))\nabla h) = sf, \tag{1.5}$$

where ϕ is the porosity function given on $Q(T)$. Since it is not easy to obtain some uniform estimates for ∇s from (1.2) in order to solve the initial boundary value problem for (1.5), we propose a new two-scale model for moisture transport. The exact form will be given in the next section. Here, we note that the model consists of two system defined on the macro and micro domains. Particularly, the system on the micro domain is a one-dimensional free boundary problem.

The two-scale model with partial differential equations was already studied by many authors, and was chosen as a mathematical model in investigations of porous media with homogenization (see [20, 24, 11, 12, 8]). We remark that both a macro and a micro systems are considered on a fixed domain in all of these results, namely, the homogeneous domain is assumed. In our model we can deal with non-homogeneous case.

The purposes of this paper are to introduce the idea of two-scale modeling for moisture transport in Section 2 and to establish the existence, uniqueness and the large time behavior of a solution of the free boundary problem in Section 3. Also, the summary is shown in the same section.

2 Two-scale model

In this section we show our two-scale model for moisture transport. Let $\Omega \subset \mathbb{R}^3$ be a bounded (macro) domain occupied with concrete, and t be the time, $0 < t < T$. We suppose that for any $\xi \in \Omega$ one pore is corresponded and regard the pore as the interval (micro domain) $(0,1)$ decomposed to the water region $(0, s(t,\xi))$ and the air region $(s(t,\xi), 1)$ (see Figure 3). Since the physical definition of the degree of saturation s is the ratio of water area to the total volume of each pore in the porous media, the degree of saturation is given by s in our formulation.

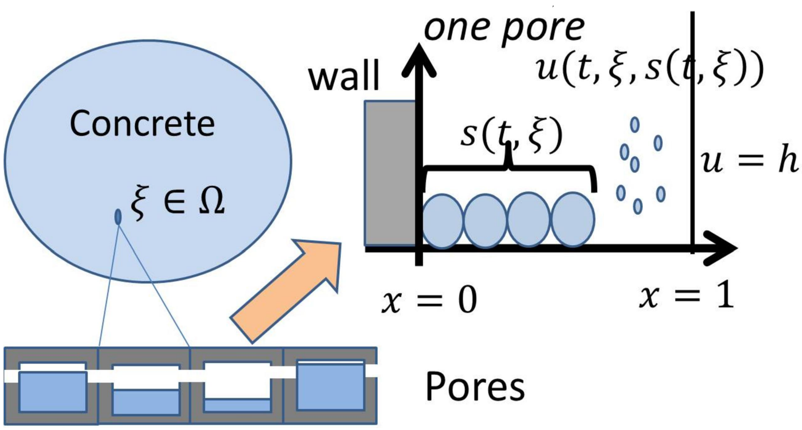

Figure 3:

Let $u(t,\xi,x)$ be the relative humidity at the place x in the air region. We impose a diffusion equation for u and the Dirichlet boundary condition at the fixed boundary $x = 1$. This boundary condition means that the air of each micro domain connects to the air of the macro domain at $x = 1$. The free boundary condition was already discussed in [22, 23, 9] so that we omit its physical interpretation. Then we can get the following free boundary problem for each $\xi \in \Omega$ and a function h on $Q(T)$: The problem FBP(h) is to find a curve $x = s(t,\xi)$, $0 \le s(t,\xi) < 1$, and a function $u(t,\xi,\cdot)$ on $(s(t,\xi),1)$ (see

Figure 4) satisfying

$$\rho_a u_t - \kappa u_{xx} = 0 \quad \text{on } (s(t,\xi),1) \text{ for } 0 < t < T, \tag{2.1}$$
$$u(t,\xi,1) = h(t,\xi) \quad \text{for } 0 < t < T, \tag{2.2}$$
$$\kappa u_x(t,\xi,s(t)) = (\rho_w - \rho_a u(t,\xi,s(t,\xi)))s'(t,\xi) \quad \text{for } 0 < t < T, \tag{2.3}$$
$$s'(t,\xi) = a(u(t,s(t,\xi)) - \varphi(s(t,\xi))) \quad \text{for } 0 < t < T, \tag{2.4}$$
$$s(0,\xi) = s_0(\xi), u(0,\xi,x) = u_0(\xi,x) \quad \text{for } s_0(\xi) \le x \le 1, \tag{2.5}$$

where ρ_a is the density of water in air, κ is a diffusion constant, the positive constant a indicates the growth rate of water region, $\varphi : \mathbb{R} \to \mathbb{R}$ is bounded and continuous, and s_0 and u_0 are initial data of s and u, respectively. Here, we give Figure 5 as a graph of the typical example of φ. Also, for each ξ we denote by S the mapping from $h(\cdot,\xi)$ to the free boundary $s(\cdot,\xi)$, namely, $S(h(\cdot,\xi)) = s$ means that s is the free boundary of the problem FBP$(h(\cdot,\xi))$.

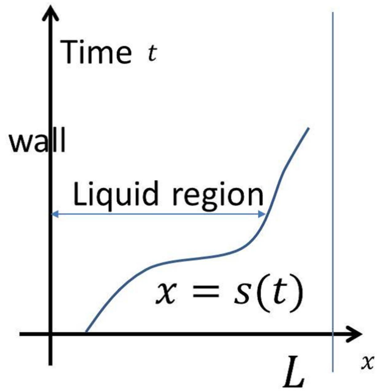

Figure 4:

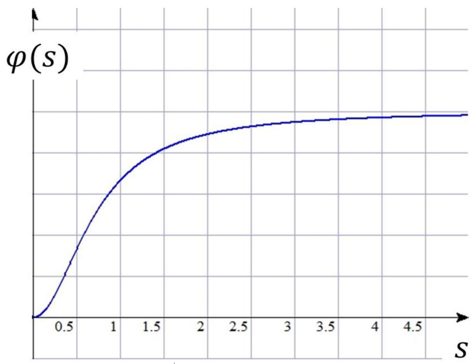

Figure 5:

Thus we obtain the two-scale model MP for moisture transport as follows: This problem is to find a triple of functions h and s on $Q(T)$ and a function u on $\Sigma_s(T) := \{(t,\xi,x) : 0 < t < T, \xi \in \Omega, s(t) < x < 1\}$ satisfying

$$\rho_w h_t - \text{ div } (g(h)\nabla h) = sf \quad \text{in } Q(T), \tag{2.6}$$
$$h = h_b \quad \text{on } \Gamma(T), \quad h(0) = h_0 \quad \text{on } \Omega, \tag{2.7}$$
$$\rho_a u_t - \kappa u_{xx} = 0 \quad \text{on } (s(t,\xi),1) \text{ for } 0 < t < T, \tag{2.8}$$
$$u(t,\xi,1) = h(t,\xi) \quad \text{for } (t,\xi) \in Q(T), \tag{2.9}$$
$$(\rho_w - \rho_a u(t,\xi,s(t,\xi)))s'(t,\xi) = \kappa u_x(t,\xi,s(t)) \quad \text{for } 0 < t < T, \tag{2.10}$$
$$s'(t,\xi) = a(u(t,\xi,s(t,\xi)) - \varphi(s(t,\xi))) \quad \text{for } (t,\xi) \in Q(T), \tag{2.11}$$
$$s(0,\xi) = s_0(\xi), u(0,\xi,x) = u_0(\xi,x) \quad \text{for } s_0 \le x \le 1, \xi \in \Omega. \tag{2.12}$$

This is the system CP with (1.2) replaced by $S(h) = s$.

3 Results on the free boundary problem and summary

In this section we show our recent results on FBP. For simplicity we omit the macro parameter ξ. First, we give assumptions for φ, a, ρ_w, ρ_a and etc.

(H1) $\varphi \in C^1(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$, $\varphi = 0$ on $(-\infty, 0]$, $\varphi \leq 1$ on $\mathbb{R}$, $\varphi'(r) > 0$ on $(0,1]$, and a is a positive constant.

(H2) ρ_w and ρ_a are positive constants with

$$\rho_w > 2\rho_a, \rho_w \geq \rho_a(|\varphi'|_{L^\infty(\mathbb{R})} + 2) \text{ and } 9a\rho_a^2 \leq \kappa\rho_w,$$

(H3) $h \in W^{1,2}_{loc}([0,\infty))$, $h' \in L^1(0,\infty) \cap L^2(0,\infty)$, $\lim_{t\to\infty} h(t) = h_\infty$, $h - h_\infty \in L^1(0,\infty)$, $0 \leq h \leq h_* < \varphi(1)$ on $(0,\infty)$, where h_* is a positive constant.

(H4) $0 \leq s_0 < 1$, $u_0 \in W^{1,2}(s_0, 1)$, $u_0(1) = h(0)$, $0 \leq u_0 \leq 1$ on $[s_0, 1]$.

Then we have proved:

Theorem 3.1. *([22, 9]) If (H1) $\sim$ (H4) hold, then the problem FBP(h) has a solution $\{s,u\}$ on $[0,\infty)$ and there exists a constant $s^* \in (0,1)$ such that $0 \leq s \leq s^*$ on $[0,\infty)$. Moreover, $s(t) \to s_\infty$ and $u(t,(1-y)s(t)+y) \to h_\infty$ for $y \in [0,1]$ as $t \to \infty$, where $s_\infty \in [0,1)$ with $\varphi(s_\infty) = h_\infty$.*

At the end of this paper, we list future works on the two-scale model for concrete carbonation.

- As mentioned in Theorem 3.1, FBP has a global solution in time. Then, since we have a chance to solve MP, we are trying it, now.
- After we solve MP, we will consider a system consisting of (1.5) and $S(h) = s$. Furthermore, we would like to deal with a couple of the system and the diffusion equation for carbon dioxide.
- Recently, we can show the existence of a periodic solution of FBP. But, the uniqueness of the periodic solution is still open. Now, we guess that it is effective to define a solution in a weak sense for its proof. However, the definition of a weak solution of FBP is not established, yet.
- We have some conjectures on the convergence rate of a solution of FBP from the observations to our numerical results in [9] so that we would like to guarantee those conjectures.

References

[1] T. Aiki, K. Kumazaki, Mathematical modeling of concrete carbonation process with hysyteresis effect. Sūrikaisekikenkyūsho Kōkyūroku, No. 1792(2012), 98-107.

[2] T. Aiki, K. Kumazaki, Mathematical model for hysteresis phenomenon in moisture transport of concrete carbonation process, Physica B, 407(2012), 1424-1426.

[3] T. Aiki, K. Kumazaki, Well-posedness of a mathematical model for moisture transport appearing in concrete carbonation process, Adv. Math. Sci. Appl., 21(2011), 361-381.

[4] T. Aiki, A. Muntean, Existence and uniqueness of solutions to a mathematical model predicting service life of concrete structures, Adv. Math. Sci. Appl., 19(2009), 109–129.

[5] T. Aiki, A. Muntean, Large time behavior of solutions to concrete carbonation problem, Communications on Pure and Applied Analysis, Vol. 9, (2010)1117-1129.

[6] T. Aiki, A. Muntean, A free-boundary problem for concrete carbonation: Rigorous justification of $\sqrt{t}$-law of propagation, Interfaces and Free Bound., 15(2012), 167-180.

[7] T. Aiki, A. Muntean, Large-time asymptotics of moving-reaction interfaces involving nonlinear Henry's law and time-dependent Dirichlet data, Nonlinear Anal., 93(2013), 3-14.

[8] T. Aiki, A. Muntean, Large-time behavior of a two-scale semilinear reaction-diffusion system for concrete sulfatation, Math. Methods Appl. Sci., 38(2015), 1451-1464.

[9] T. Aiki, Y. Murase, On a large time behavior of a solution to a one-dimensional free boundary problem for adsorption phenomena, in preparation.

[10] M. Brokate and J. Sprekels, *Hysteresis and Phase Transitions*, Springer, Appl. Math. Sci., 121, 1996.

[11] V. Chalupecký, T. Fatima, and A. Muntean. Numerical study of a fast micro-macro mass transfer limit: The case of sulfate attack in sewer pipes. *J. of Math-for-Industry*, 2B:171–181, 2010.

[12] T. Fatima, A. Muntean and T. Aiki. Distributed space scales in a semilinear reaction-diffusion system including a parabolic variational inequality: A well-posedness study, Adv. Math. Sci. Appl. 22(2012), 295-318.

[13] K. Kumazaki, A mathematical model of carbon dioxide transport in concrete carbonation process. Discrete Contin. Dyn. Syst. Ser. S 7 (2014), no. 1, 113—125.

[14] K. Kumazaki, Large time behavior of a solution of carbon dioxide transport model in concrete carbonation process. J. Differential Equations, 257(2014), 2136-2158.

[15] K. Kumazaki, Exponential decay of a solution for some parabolic equation involving a time nonlocal term, Math. Bohem., 140(2015), 129-137.

[16] K. Kumazaki, T. Aiki, Uniqueness of a solution for some parabolic type equation with hysteresis in three dimensions. Networks and Heterogeneous Media, 9(2014), 683-707.

[17] K. Maekawa, R. Chaube, T. Kishi, *Modeling of concrete performance*, Taylor and Francis, 1999.

[18] K. Maekawa, T. Ishida, T. Kishi, Multi-scale modeling of concrete performance, Journal of Advanced Concrete Technology, 1(2003), 91-126.

[19] A. Muntean, A moving-boundary problem: Modeling, analysis and simulation of concrete carbonation, Cuvillier Verlag, Götingen, 2006. PhD thesis, Faculty of Mathematics, University of Bremen, Germany.

[20] A. Muntean and M. Neuss-Radu, A multiscale Galerkin approach for a class of nonlinear coupled reaction-diffusion systems in complex media, J. Math. Anal. Appl., 371(2010), 705–718.

[21] A. Muntean, M. Böhm, A moving-boundary problem for concrete carbonation: global existence and uniqueness of solutions, Journal of Mathematical Analysis and Applications, 350(1)(2009), 234-251.

[22] N. Sato, T. Aiki, Y. Murase, K. Shirakawa, A mathematical model for a hysteresis appearing in adsorption phenomena, Sūrikaisekikenkyūsho Kōkyūroku, No. 1856(2013), 1-11.

[23] N. Sato, T. Aiki, Y. Murase, K. Shirakawa, A one dimensional free boundary problem for adsorption phenomena, Netw. Heterog. Media, 9(2014), 655-668.

[24] T. Fatima and N. Arab and E. P. Zemskov and A. Muntean, Homogenization of a reaction-diffusion system modeling sulfate corrosion in locally-periodic perforated domains, J. Eng. Math., 69(2011), 261–276.

[25] A. Visintin, *Differential Models of Hysteresis*, Appl. Math. Sci., Vol. 111, Springer-Verlag, Berlin, 1993.